Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Spectroscopic and Quantum-Chemical Study of Structure of Liquid Crystalline Cyanobiphenyls and Arylcyanopyridines

V. T. Grachev [a], B. E. Zaitsev [a], E. M. Itskovich [a], A. I. Pavluchenko [a], N. I. Smirnova [a], V. V. Titov [a] & K. M. Dyumaev [a]

[a] Organic Intermediates and Dyes Institute, Moscow, K-I, U.S.S.R.

Version of record first published: 20 Apr 2011.

To cite this article: V. T. Grachev , B. E. Zaitsev , E. M. Itskovich , A. I. Pavluchenko , N. I. Smirnova , V. V. Titov & K. M. Dyumaev (1981): Spectroscopic and Quantum-Chemical Study of Structure of Liquid Crystalline Cyanobiphenyls and Arylcyanopyridines, Molecular Crystals and Liquid Crystals, 65:1-2, 133-144

To link to this article: http://dx.doi.org/10.1080/00268948108076135

Mol. Cryst. Liq. Cryst., 1981, Vol. 65, pp. 133–144
0026-8941/81/6502–0133$06.50/0

Spectroscopic and Quantum-Chemical Study of Structure of Liquid Crystalline Cyanobiphenyls and Arylcyanopyridines

V. T. GRACHEV, B. E. ZAITSEV, E. M. ITSKOVICH, A. I. PAVLUCHENKO, N. I. SMIRNOVA, V. V. TITOV, and K. M. DYUMAEV

Organic Intermediates and Dyes Institute, Moscow K-1, U.S.S.R.

(*Received January 22, 1980; in final form May 15, 1980*)

Under study were the UV and PMR spectra as well as the electron structure of 4-alkyl, 4-alkoxy-4′-cyanobiphenyls, 6-*p*-alkylphenyl-, 6-*p*-alkoxyphenyl-3-cyanopyridines and 5-alkyl-2-*p*-cyanophenylpyridines in the ground and first excited states. To study these compounds a quantitative method is offered for determination the rotation angle between the planes of bicyclic molecular fragments based on the excitation theory within the frames of the Hückel technique and on the UV spectroscopy data.

INTRODUCTION

The present investigation is aimed at the experimental and theoretical examination of peculiar structure features of some biphenyl and arylpyridine derivatives. Such a complex approach to the study of different classes of mesomorphic compounds with sufficient statistical material available should provide an opportunity for predicting certain structures of liquid crystalline compounds with useful properties.

EXPERIMENTAL

Electron absorption spectra (Table II) have been recorded with a spectrophotometer Specord UV/Vis at concentrations 10^{-4} to 10^{-5} mole/l. The PMR spectra have been taken with a spectrophotometer Varian-HA 100D at 21°C in CCl_4 (Table IV) with GMDS used as an internal etalon.

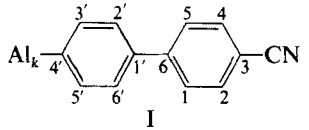
The quantum chemistry of ground and first excited states of the neutral forms of compounds I–V was examined through the LCAO MO technique in the PPP approximation, taking into account the configuration interaction, following the programme based upon the Dewar algorithm.[5] The computations assumed that the molecules were planar and the valence angles were near 120°. The lengths of the bonds

$C{=}C$, $C{=}N$, $>C-C\equiv$, $>C-C<$, $C\equiv N$, $C-CH_3$ and $C-O$

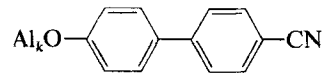
were thought to be equal to 1.39; 1.39; 1.419; 1.49; 1.158; 1.51 and 1.34 Å respectively. The ionization potentials (I_p), the concentric Coulomb integrals (γ_{pp}) and the resonance ones (β_{pg}) for the atoms (Table VI) have been found through the theory of perturbation from the transition energy values ΔE_n of the absorption bands in the electron spectra of the π-systems containing this atom. The technique to determine the parameters of I_p, γ_{pp} and β_{pg} will be described in more details in a separate paper. The Coulomb (g_r) and resonance (k_{rs}) parameters (Table VII) were found by the technique described in our paper[3] and have been used to computate the θ angle in compounds I–V (Table VII) through the perturbation theory within the frames of the MOH method.

RESULTS AND DISCUSSIONS

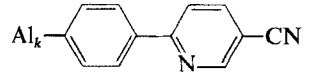
When studying the structure of 4-alkyl-(I), 4-alkoxy-4-cyanobiphenyls (II), 6-*p*-alkylphenyl-(III), 6-alkoxyphenyl-3-cyanopyridines (IV) and 5-alkyl-2-*p*-cyanophenylpyridines (V), it is interesting to calculate the rotation angle (θ) between the planes of a benzonitrile or a 3-cyanopyridine fragment and the phenyl group in the compounds I–V. It can be obtained from UV spectroscopy data.



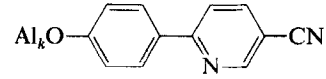
I



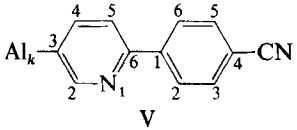
II



III



IV



V

The technique to determine the θ angle is based upon the idea that the maximum (ΔE_1) of the long-wave band π–π^* in the electron absorption spectrum of the π-system basically depends on the transition of π-electron in the upper occupied molecular orbital (E_{uomo}) onto the lower one which is free (E_{lfmo}):

$$\Delta E_1 = (E_{\text{lfmo}} - E_{\text{uomo}}) \cdot \beta \tag{1}$$

Dewar has used the perturbation theory (PT) within the frames of the Hückel MO technique for his examination of the interactions between the π-conjugate systems (I). A formation of the bond R—S between the π-systems R—S is typical for its resonance integral $\beta_{rs} = K_{\text{RS}} \cdot \beta$ between the terminal AO χ_r and χ_s which is regarded as a perturbation. The interaction between the π-systems R and S is comprised of the pair interactions of the individual levels E_n^R and E_k^S MO $\psi_n^R = \sum_r a_n, r \cdot \chi_R$ and $\psi_k^S = \sum_s B_{k,s} \cdot \mathrm{X}_s$. Hereby the upper level of the E_n^R and E_k^S goes up whilst the lower one goes down by the same value (with $E_n^R \neq E_k^S$):

$$\frac{a_{n,r}^2 \cdot b_{k,s}^2}{E_n^R - E_k^s} \cdot k_{rs}^2 \cdot \beta \tag{2}$$

If among the values of E_n^R and E_k^S happen to be equal ones ($E_n^R = E_k$) their interactions result in the appearance of the following levels:

$$\begin{aligned} E_n^{R'} &= E_n^R + a_{n,r} \cdot b_{k,s} \cdot k_{rs} \cdot \beta \\ E_k^{S'} &= E_k^S - a_{n,r} \cdot b_{k,s} \cdot k_{rs} \cdot \beta \end{aligned} \tag{3}$$

In this case the splitting is of the first order in the value of k_{rs}. It is a general rule: the closer the levels are to each other, the stronger is their interaction.

It is necessary to find out now which of the levels E_{n+k}^{RS} will be E_{uomo}^{RS} and E_{lmfo}^{RS} in the new RS system. If the E_{uomo}^{RS} and E_{lmfo}^{RS} are equal to the values of the excited $E_{\text{uomo}}^R = E_{\text{m}}^R$ and $E_{\text{lfmo}}^R = E_{\text{m}+1}^R$ of the R system, it will be the only case to show the effect of the π-system S upon the maximum ΔE_1^R of the long-wave absorption band of the R system. It is possible if

$$|E_m^R| < |E_m^S|, |E_{m+1}^R| < |E_{m+1}^S| \tag{4}$$

which follows from expressions (2–3). Then Eq. (1), according to (2), with the nongenerate system R and S and $E_n^R \neq E_k^S$ will look like

$$\Delta E_1^{RS} = \Delta E_1^R + \sum_k \left(\frac{a_{m+1,r}^2 \cdot b_{k,s}^2}{E_{m+1}^R - E_k^s} - \frac{a_{m,r}^2 \cdot b_{k,s}^2}{E_m^k - E_k^s} \right) \cdot k_{rs} \cdot \beta \tag{5}$$

where $E_1^R = (E_{m+1}^R - E_m^R) \cdot \beta$.

If we complete the inequalities

$$|E_m^R| < |E_m^S| \quad \text{and} \quad |E_m^R| > |E_m^S| \tag{6}$$

the long-wave absorption band in the *RS* joint spectrum will depend on the transition of the π-electron with the excited UOMO of the *R* system onto the excited LFMO of the *S* system (or the transition of the charge from the *R* system to the *S* system). In this case Eq. (1) will be the following:

$$\Delta E_1^{RS} = (E_{m+1}^S - E_m^R) \cdot \beta + \left(\sum_n \frac{b_{m+1,s}^2 \cdot a_{n,r}^2}{E_{m+1}^S - E_n^R} - \sum_k \frac{a_{m,r}^2 \cdot b_{k,s}^2}{E_m^R - E_k^S} \right) \cdot k_{rs}^2 \cdot \beta \quad (7)$$

Substituting the experimental values of ΔE_1^{RS} and ΔE_1^R in Eqs. (5) and (7), we can calculate the value of k_{rs}. According to Refs. 1, 2, the equality $k_{rs} = \cos\theta$ is the rotation angle in question. Equations 1–3, 5 and 7) include the resonance integral β for the C=C bond in benzene. This bond can be easily found from Eq. (1). When for benzene $\Delta E_1 = 4.88$ eV, it is $\beta = -2.44$ eV.

When using Eqs. (1, 5 and 7), it is necessary by means of the technique described herein[3] to select first the values of the Coulomb and resonance parameters in such a way that the values of ΔE_1^R and ΔE_1^S found through the MOH technique ahould coincide with the experimental ones. Equations (5) and (7) may be used only in case of PT. In other cases the values of k_{rs} are to be found by the method of successive approximations. When comparing the MO-LCAO-computed Pariser-Parr-Pople (PPP) cite reference approximated transition energies and oscillator powers with the experimental data of the UV spectroscopy of compounds I–V, and when analyzing the coefficients $(A_n i - j)$ of the configurative interaction matrices (Table I), one can see that in the neutral forms of compounds similar to those from I to V the long-wave absorption band by 89–90% depends on the singlet-singlet transition of the π-electron from the UOMO onto the LFMO.

Hence, the technique offered earlier for determining the θ angle between the planes of the fragments is also applicable to compounds I–V. Alkylbenzenes, alkoxybenzenes and 3-alkylpyridines have been taken here as a *R*-system, benzonitrile and 3-cyanopyridine as a *S*-system, and compounds of the I–V type as a *RS*-system. Since the UV-absorption spectra of

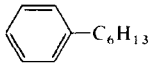
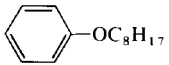
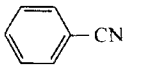
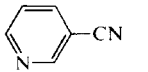
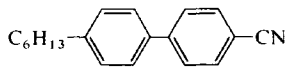
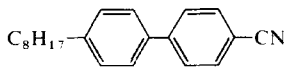
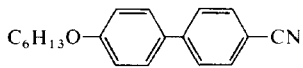
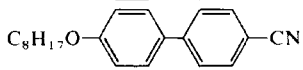
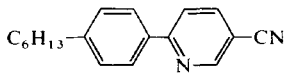
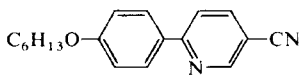
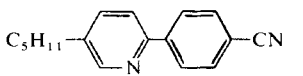
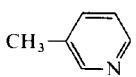
TABLE I

Calculated and experimental data on the long-wave absorption band in the electron spectra of neutral forms of compounds I-V

Type of compound	Calculations				Experiments	
	ΔE_I (ev)	f_1	α_0	$An(i \to j)$	ΔE_I^{max} (ev)	ε_I^{max}
I	4.24	1.130	−30	0.97(8–9)	4.30	77250
II	4.13	1.095	−30	0.97(8–9)	4.14	82600
III	3.91	0.996	−32	0.94(8–9)	4.08	51600
IV	3.83	0.999	−32	0.95(8–9)	3.82	63200
V	4.18	0.982	−39	0.94(8–9)	4.28	20380

TABLE II

UV-spectroscopy data (in ethanol)

Compound	λ_n^{max} (nm)								ε_n^{max}							
	211	245*	250*	255*	260*	263*	266*	269*	9000	196	225	243	270	287	199	216
	205*	222*	264*	271	278*				3660	5600	900	1175	760	1050	990	
	202	223*	227*	231*		263*	270*	278*	8400	15600	1520	1320	760	1069	990	
	216	261*	267*	273*		306			11500	2900	3280		2430	1250		
	208*	216*	288						67500	57200		77250				
	208*	216*	286						59600	53600		72250				
	206	223	298						54200	45100		61700				
	207	225	300						60250	58400		82600				
	207*	216*	274*		302*				31200	32000		31600		51600		
	205	222	325						29600	30100		6320				
	208	265	290						21800	18100		20380				
		266								3100						

* Shoulder.

alkyl benzenes and alkoxybenzenes as well as those of compounds I–V practically do not depend upon the size of the alkyl and alkoxy groups (Table II), we used the data on the UV spectroscopy and the ionization potentials of toluene and phenol in our theoretical and experimental evaluations of E^R_{uomo} and E^R_{lfmo} (Table III).[4]

The analysis of the calculated values of UOMO and LFMO of the *R* and *S* systems (Table III) shows that $|E^R_{\text{uomo}}| < |E^S_{\text{uomo}}|$, and $|E^R_{\text{lfmo}}| > |E^S_{\text{lfmo}}|$. Hence, in this case inequalities (6) are satisfied and in the electron spectra of compounds I–V the absorption maximum E^{RS}_1 depends on the charge transition (Eq. (7)) from the UOMO of the aklylbenzene, alkoxybenzene and 3-alkylpyridine fragments on the LFMO of benzonitrile or 3-cyanopyridine respectively. According to our calculations, the θ angle for compounds I and II is equal to 84° and 75°, for compounds III and IV— to 66° and 53° and

TABLE III

Calculated and experimental values of UOMO, LFMO, ΔE_1 and J for compounds under study and their fragments in e.v.

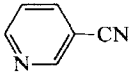
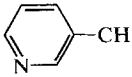
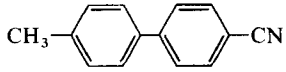
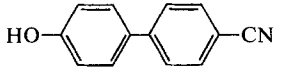
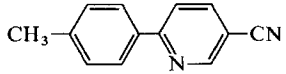
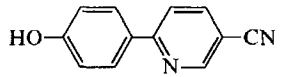
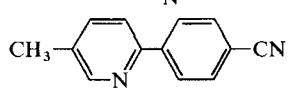
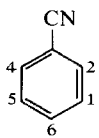
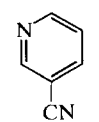
Compound	Calculations					Experiments		
	$\times\beta$ LFMO	$\times\beta$ UOMO	J_{ev}	$\times\beta$ ΔE_1	λ_1 (nm)	J_{ev}	$\times\beta$ ΔE_1^{max}	λ_1^{max} (nm)
Ph—CH_3	−1.0	0.928	9.07	1.93	263	8.82 9.20	1.93	263
Ph—OH	−1.0	0.879	8.95	1.88	271	9.03	1.88	271
Ph—CN	−0.821	0.999	9.24	1.82	278	9.71	1.82	278
	−0.901	0.999	9.24	1.90	267	—	1.90	267
	−0.940	0.950	9.11	1.89	266	9.04	1.89	266
	−0.820	0.927	9.07	1.75	287	—	1.76	288
	−0.810	0.867	8.92	1.68	300	—	1.68	300
	−0.825	0.845	8.87	1.67	302	—	1.67	302
	−0.784	0.764	8.68	1.56	325	—	1.56	325
	−0.816	0.933	9.08	1.75	290	—	1.75	290

TABLE IV

Chemical shifts of ring protons (m.p.) and distribution of -electron density (q_r) for neutral forms of compounds I-V in the basic (q_r^0) and Its excited states (q_r^1)

Compound	Calculation technique	Chemical shift	Fragments C_6H_5Alk or C_5N_4NAlk							Fragments C_6H_5CN or C_5H_4NCN						C≡N	
			C_1	C_2	C_3	C_4	C_5	C_6	CH_3	C_1	C_2	C_3	C_4	C_5	C_6	C	N
		c.s.		7.34	7.11		7.11	7.34		7.50	7.50		7.50	7.50			
	MOH	q_r^0	1.010	0.999	1.016	0.982	1.015	0.999	1.980	1.001	0.979	1.018	0.979	1.001	0.984	0.534	1.501
I	PPP	q_r^0	1.053	0.983	1.086	0.884	1.086	0.983	1.888	1.008	0.971	1.048	0.971	1.008	0.966	0.635	1.431
	PPP	q_r^0	0.906	0.977	1.032	0.821	1.032	0.977	1.865	0.973	10032	1.072	1.032	0.973	1.064	0.752	1.492
		c.s.		7.34	6.81		6.81	7.34		7.50	7.50		7.50	7.50			
	MOH	q_r^0	1.018	0.998	1.024	0.973	1.024	0.998	1.980	1.001	0.979	1.018	0.979	1.001	0.984	0.537	1.501
II	PPP	q_r^0	1.025	0.990	1.031	0.988	1.031	0.990	1.922	1.003	0.970	1.042	0.970	1.003	0.971	0.635	1.428
	PPP	q_r^0	0.921	0.984	0.996	0.940	0.996	0.984	1.859	0.977	1.022	1.054	1.022	0.977	1.046	0.742	1.481
		c.s.		7.83	7.14		7.14	7.83		8.75			7.79	7.65			
III	MOH	q_r^0	1.011	0.998	1.015	0.981	1.015	0.998	1.980	1.081	0.961	1.009	0.973	1.002	0.964	0.517	1.496
	PPP	q_r^0	1.063	0.969	1.090	0.871	1.086	0.946	1.875	1.477	0.761	1.077	0.890	1.032	0.783	0.637	1.432
	PPP	q_r'	0.906	0.992	1.032	0.821	1.048	0.942	0.866	1.572	0.702	1.042	1.097	0.860	0.988	0.685	1.448
		c.s.		7.76	6.81		6.81	7.76	8.72		8.72		7.76	7.59			
IV	MOH	q_r^0	1.018	0.996	1.024	0.971	1.024	0.996	1.962	1.083	0.961	1.009	0.973	1.003	0.965	0.538	1.474
	PPP	q_r^0	1.036	0.976	1.035	0.976	1.032	0.953	1.919	1.473	0.760	1.072	0.887	1.028	0.786	0.638	1.429
	PPP	q_r'	0.923	1.005	0.991	0.936	1.014	0.942	1.872	1.574	0.681	1.029	1.088	0.845	0.968	0.682	1.442
		c.s.		7.50	7.62		7.62	7.50			8.46		8.07	7.64			
V	MOH	q_r^0	0.984	1.001	0.979	1.018	0.979	1.001	1.980	1.078	0.983	0.984	0.994	1.001	0.979	0.537	1.501
	PPP	q_r^0	0.979	0.995	0.975	1.035	0.972	0.982	1.892	1.457	0.874	0.915	1.000	1.009	0.865	0.635	1.427
		q_r'	1.001	1.004	0.986	1.041	1.007	0.938	1.864	1.587	0.887	0.833	1.098	0.856	0.862	0.685	1.453
	MOH	q_r^0								1.001	0.979	1.018	0.979	1.001	0.984	0.537	1.501
	PPP	q_r^0								0.996	0.969	1.036	0.969	0.996	0.974	0.634	1.425
	MOH	q_r^0								1.080	0.961	1.008	0.973	1.002	0.963	0.517	1.496
	PPP	q_r^0								1.453	0.759	1.060	0.879	1.021	0.768	0.637	1.423

* Scale (m.p.), internal standard GMDS, solvent CCl_4.

for compounds V— to 84° respectively. Thus, if we introduce an N atom into the 3d position of benzonitrile in compounds I–II, the rotation angle θ will decrease by 20° due to the increased electron acceptability (and, consequently, π-conjugation) of a heterocycle with a phenyl ring. When a nitrogen atom is introduced in the 3d position of alkylbenzenes in compounds of the I type, the electron acceptive properties of the two fragments (in compounds of type V) level up and the θ value does not undergo great changes.

It should be noted that the completed condition of $|E_m^R| < E_m^S|$ guarantees that the ionization potential I^{RS} in the bicyclic compounds of type I–V will be always lower than the minimal one of the two ionization potentials I^R and I^S of the π-conjugate fragments R and S (Table III), the difference showing the value of interactions between the level E_m^R and all the E_k^S levels:

$$I^{RS} = I^R - \sum_k \frac{a_{m,r}^2 \cdot b_{k,s}^2}{E_m^R - E_k^S} \cdot k_{rs}^2 \cdot \beta$$

Let us now consider the specific electron structure of compounds similar to the type I–V. To prove the validity of our calculations of the π-electron density distribution (q_r) in compounds I–V we can point to the fact that the sequence in the location of the chemical shears (CS) of the ring protons coincides with that of the q_r values on the respective carbon atoms (Table IV). And, indeed, the sequences of the increasing chemical shears for compounds I–II such as $H'_3 = H'_5 < H_2 = H'_6 < H'_2 = H_6$ are similar to the sequences of the decreases q_r values: $q'_3 = q'_5 > q_2 = q'_6 > q'_2 = q_6$ or $q'_3 = q'_5 > q'_1 = q'_5 > q'_2 = q'_6 > q_2 = q_6$; in compounds III–IV the sequences of $H'_3 = H'_5 < H_5 < H_4 < H'_2 = H'_6 < H_2$ correpond to those of $q'_3 = q'_5 > q_5 > q'_2 = q'_6 > q_2$; in compound V for the benzene cycle $H'_2 = H'_6 < H'_3 = H'_5$ we find as corresponding the sequence $q'_2 = q'_6 > q'_3 = q'_5$, while for the 3-alkylpyridine cycle the sequences $H_5 < H_4 < H_2$ corresponds to that of $q_5 > q_4 > q_2$. It should be noted that the q_r values found through the MO techniques in the PPP and MOH approximations are close to one another (Table IV). In the ground state of compounds I–II the sum negative π-electron charge ($\Sigma_r Q_r$) is in the benzonitrile fragment, and is equal to -0.055 (see q_r calculated through the PPP technique in Table IV); in compounds III–IV it is concentrated in the 3-cyanopyridine fragment and is equal to -0.099 and in compounds of type $V \Sigma_r Qr = -0.003$ in the benzonitrile part. Thus, in compounds I–IV the benzonitrile and 3-cyanopyridine fragments act as π-electron acceptors. It is interesting to note that in 3-cyanopyridines this property seems to be twice as strong as it is in benzonitriles. Compounds of type V do not reveal a benzonitrile to be a stronger π-electron acceptor than a 3-alkylpyridine is.

TABLE V

Calculated dipole moments in (D) for compounds of type I–V

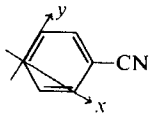
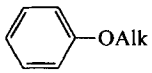
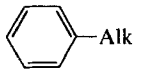
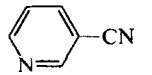
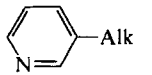
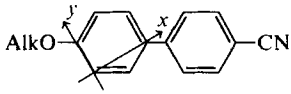
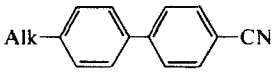
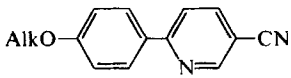
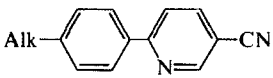
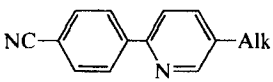
Type of compound	Basic state μ_π	α°_μ	μ_x	μ_y	1st excited state μ'_π	α°
	3.297	+30	2.942	0.699	5.755	+30
	0.864	−30	−0.748	−0.432	2.492	−30
	0.860	−30	−1.611	−0.930	2.253	−30
	2.943	−8	2.926	−0.401	3.248	9
	3.419	−62	−0.608	−3.018	3.748	−53
	4.936	−30	4.245	−2.468	14.045	−30
	6.311	−30	5.465	−3.155	16.342	−30
	5.594	−49	3.321	−3.862	10.327	−39
	6.477	−45	4.573	−4.582	12.451	−37
	6.668	15	−6.436	0.745	11.286	+19

TABLE VI

Ionization potentials (J_p), concentric Coulomb (γ_{pp}) and resonance (β_{pq}) integrals for atoms in the PPP technique

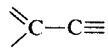
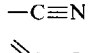
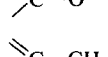
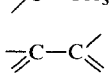
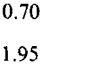
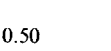
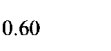
Atom (p)	I (p)	γ_{pp}	p–q	β_{pq}
—Ċ—	11.13	11.16	C═C	−2.39
—Ċ≡	11.13	11.16	C═N	−2.58
—N—	17.00	12.34		−2.00
—Ṅ≡	17.00	12.34	—C≡N	−3.5
Ö	44.51	34.25		−1.54
CH_3	29.0	10.00		−5.00
				cos θ β C═C

TABLE VII

Coulomb (h_r) and resonance (k_{rs}) parameters to calculate compounds of type through MOH technique

Atom (r)	h_r	r-s bond	k_{rs}	Compound	$k_{c-c=}\cos\theta$	θ
—Ṅ═	0.20	C═C═N	1.00	I	0.1	84
Ṅ≡	0.99		0.70	II	0.3	75
—Ċ≡	−0.60	—C≡N	1.95	III	0.4	66
CH_3	2.27		0.50	IV	0.6	53
Ö	1.84		0.60	V	0.1	84

In the first excited state of compounds I–II, V and III–IV the negative values of $\Sigma_r Q_r$ are concentrated in the benzonitrile and 3-cyanopyridine fragments; they are equal to −0.342, −0.069 and −0.305 respectively. Hence, in this case the π-electron charge transfer from the electron donor to the electron acceptor increases considerably.

In the ground state the π-dipole moments (μ_π^0) of compounds I–II are smaller than the μ_π^0 of compounds III–IV, whilst in the first excited state it is vice versa (Table V). It is interesting to note that in compounds I–II the directions (α_0) of the vectors μ_π^0 and μ_π' do not undergo any changes thanks to the symmetry axis along the molecule (Table V).

References

1. M. J. S. Dewar, *J. Am. Chem. Soc.*, **74**, 3341 (1952).
2. J. Fisher-Hjalmors, *Arkiv Fisic*, **21** 123 (1962).
3. V. T. Grachev, B. E. Zaitsev, P. B. Terentyev, N. P. Lomakina, and K. M. Djumaev, *Khim. Geterotskii Soed.*, 1243, 1975.
4. L. V. Gurvich, G. V. Karachevtsev, V. N. Kondratyev, Y. A. Lebedev, V. A. Medvedev, V. K. Potapov, and Y. S. Khodyeev, *Energies of chemical bond breaking. Ionization potentials and electron affinity*, ed., "Nauka," Moscow, 1974.
5. M. J. S. Dewar, *The Molecular Orbital Theory of organic chemistry*, McGraw Hill Company, New York, New York, 1969.